Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Online Material for

Computational Study of H_2 binding to MH_3 (M= Ti, V, and Cr)

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Supporting Materials:

Figures S1-S2

Table S1

Geometry Data Tables S2 – S5

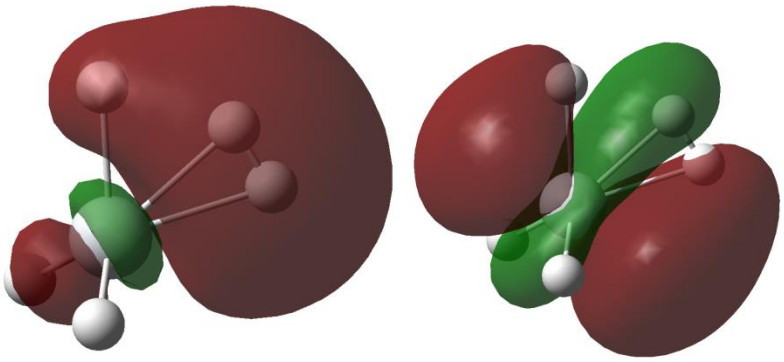

Figure S1. The orbitals that are involved in the complexation of H_2 on TiH_3. Left: HOMO, and Right: HOMO-4. These orbitals are displayed with an isovalue of 0.02 a.u.

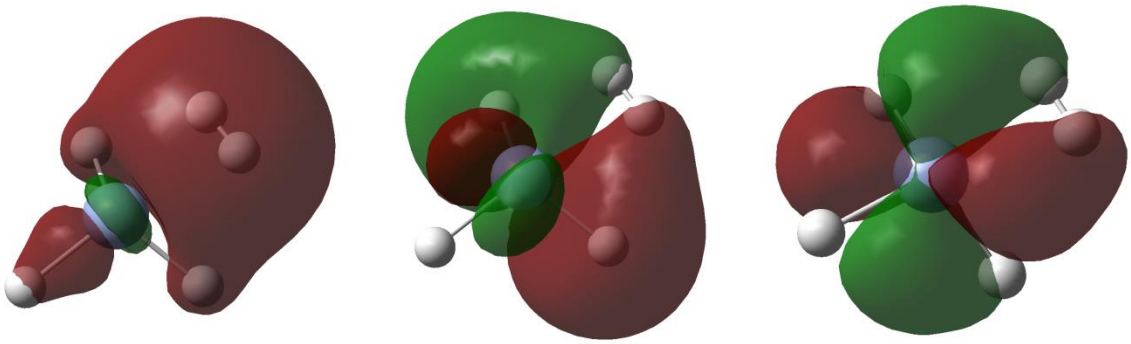

Figure S2. The orbitals that are involved in the complexation of H_2 on CrH_3. Left: HOMO-2, Centre: HOMO-4, and Right: HOMO-6. These orbitals are displayed with an isovalue of 0.02 a.u.

Table S1. Individual H-H Bond Distances (Å) and Stretching Frequencies ($\bar{\nu}$, cm^{-1}) for the Maximum Loading of H_2 bound to the base structure on M_5H_{15} (M=Ti, and V) and Cr_5H_{11}.

Ti_5H_{15} + nH_2	d_{H-H} H_2	d_{M-H2}	Stretching Frequency	V_5H_{15} + nH_2	d_{H-H} H_2	d_{M-H2}	Stretching Frequency	Cr_5H_{11} + nH_2	d_{H-H} H_2	d_{M-H2}	Stretching Frequency
	0.844	1.903	2943		0.866	1.784	2738		0.879	1.721	2612
	0.843	1.895	2964		0.854	1.817	2838		0.877	1.724	2636
	0.841	1.916	2982		0.828	1.870	3144		0.844	1.797	2981
	0.813	1.964	3342		0.825	1.844	3212		0.815	1.816	3319
	0.805	1.976	3452		0.815	1.848	3338		0.807	1.854	3430
	0.799	2.001	3552		0.800	1.913	3542		0.775	2.096	3916
	0.786	2.057	3731		0.795	1.927	3615		0.755	3.379	4227
15	0.780	2.069	3834	13	0.756	3.448	4184	12	0.755	3.197	4236
	0.779	2.067	3865		0.754	3.524	4215		0.754	3.388	4244
	0.755	3.734	4200		0.754	3.692	4225		0.753	4.082	4251
	0.755	3.976	4217		0.754	3.715	4230		0.754	3.672	4252
	0.754	3.878	4220		0.754	3.773	4233		0.754	3.551	4254
	0.754	3.835	4228		0.754	4.102	4233				
	0.753	4.089	4242								
	0.754	4.186	4245								
R^2	d_{H-H} and d_{M-H2}: 0.70	d_{H-H} and $\bar{\nu}$: 1.00	d_{M-H2} and $\bar{\nu}$: 0.73	R^2	d_{H-H} and d_{M-H2}: 0.81	d_{H-H} and $\bar{\nu}$: 1.00	d_{M-H2} and $\bar{\nu}$: 0.84	R^2	d_{H-H} and d_{M-H2}: 0.73	d_{H-H} and $\bar{\nu}$: 0.99	d_{M-H2} and $\bar{\nu}$: 0.78

Computational Geometry Data

Systems that are optimised to the Default criteria as opposed to VeryTight are marked with **

Table S2. Cartesian Coordinates of H_2 Optimized Geometry: SCF Energy

H_2, -1.1658575

H 0.000000 0.000000 0.375989
H 0.000000 0.000000 -0.375989

Table S3. Cartesian Coordinates of $MH_3.nH_2$ (M = Ti, V, and Cr) Monomers Optimized Geometry: SCF Energy, *Hydrogen Binding Energy (kJ mol^{-1}),* **Hydrogen Binding Gibbs Free Energy (kJ mol^{-1})**

TiH_3, -850.898907

Ti 0.000000 0.040940 0.000000
H 1.698087 -0.300184 0.000000
H -0.849043 -0.300245 1.470588
H -0.849043 -0.300245 -1.470588

VH_3, -945.4297849

V 0.000000 0.009108 0.000000
H 1.675052 -0.069746 0.000000
H -0.837526 -0.069871 1.450631
H -0.837526 -0.069871 -1.450631

CrH_3, -1045.913751

Cr 0.000000 0.069235 0.000000
H 1.490575 -0.553871 0.000000
H -0.745288 -0.553881 1.290872

H -0.745288 -0.553881 -1.290872

$TiH_3.H_2$, -852.0785716, *-36.3*, **5.9**

Ti -0.108634 0.000000 0.000329
H -0.995575 -1.485872 0.159641
H -0.995572 1.485873 0.159643
H 0.994652 0.000000 -1.339747
H 1.614645 -0.000002 0.916260
H 1.771788 0.000000 0.096967

$VH_3.H_2$, -946.6153761, *-51.8*, **-9.2**

V 0.000000 0.151875 0.000000
H -1.672809 0.138783 -0.000000
H 0.736781 -0.177143 1.468504
H 0.736781 -0.177143 -1.468504
H 0.099623 -1.638807 0.404965
H 0.099623 -1.638807 -0.404965

$CrH_3.H_2$, -1047.088784, *-24.1*, **13.8**

Cr 0.000000 0.118028 0.000000
H 0.813238 1.532557 0.000000
H 0.526488 -0.606965 1.346945
H 0.526488 -0.606965 -1.346945
H -0.933107 -1.575655 0.393052
H -0.933107 -1.575655 -0.393052

$TiH_3.5H_2$, -856.8063699, *-41.1*, **2.1**

Ti 0.010982 -0.003105 -0.017012
H -0.582739 0.641544 -1.524266
H -0.331411 -1.153036 -1.279958
H -0.472601 0.133689 1.689438
H 1.691615 0.410360 1.030022
H 1.079901 0.346544 1.557498
H -1.865848 -0.132078 0.545031
H -1.932128 -0.182455 -0.249729
H 0.050097 -1.707622 0.867654
H -0.067253 -1.879834 0.059951
H 1.563167 -0.410815 -1.104807
H 1.526921 0.398634 -1.167943

H -0.390524 1.841653 0.384640
H -0.510801 1.761724 -0.433278

$VH_3.4H_2$, -950.1769539, *-55.0*, **-11.2**

V 0.000001 -0.000002 -0.003331
H -0.000078 -0.000003 1.692626
H -0.000599 0.920476 -1.407935
H 0.000697 -0.920486 -1.407931
H 1.875130 0.001271 0.364510
H 1.854842 0.001227 -0.432579
H -0.001148 1.629175 0.757289
H -0.001225 1.786789 -0.089203
H -1.854823 -0.001193 -0.432667
H -1.875142 -0.001248 0.364421
H 0.001226 -1.786790 -0.089204
H 0.001086 -1.629176 0.757290

$CrH_3.3H_2$, -1049.466147, *-48.0*, **-5.1**

Cr 0.000005 -0.048250 -0.083401
H 0.458535 -1.524582 0.661717
H -0.458430 -1.524621 0.661699
H -0.000035 1.310736 -1.024578
H -1.721424 -0.260588 -0.146342
H -1.529696 0.481516 -0.595832
H 1.529680 0.481651 -0.595768
H 1.721455 -0.260437 -0.146270
H -0.000100 0.942352 1.855567
H -0.000108 1.511964 1.331437

Table S4. Cartesian Coordinates of $MH_3.nH_2$ (M = Ti, V, and Cr) Dimers, M_2H_6**,** Optimized Geometry: SCF Energy, *Hydrogen Binding Energy (kJ mol^{-1}),* **Hydrogen Binding Gibbs Free Energy (kJ mol^{-1})**

Ti_2H_6, -1701.891545

H 0.000000 -0.000674 -1.440484
H -0.000001 -0.989435 0.774708
H 2.144578 -1.360400 0.522853
H -2.144570 -1.360400 0.522861
H 1.550316 1.544913 0.716459

H -1.550313 1.544917 0.716455
Ti 1.266840 0.014116 -0.041201
Ti -1.266840 0.014115 -0.041201

V_2H_6, -1890.959635

H -0.038400 -0.570044 -1.191155
H -0.038403 -0.570059 1.191146
H 2.112653 -1.418913 0.000003
H -2.961724 0.079519 0.000011
H 1.915208 1.506161 0.000003
H -0.168912 1.330329 0.000008
V 1.207278 0.001522 0.000000
V -1.242949 -0.017044 -0.000001

Cr_2H_6, -2091.90742

H 0.094044 -0.623859 1.077624
H 0.094058 -0.623944 -1.077574
H -2.805813 0.407042 0.000013
H 2.591966 -0.935775 -0.000011
H -2.234899 1.173622 -0.000012
H -0.267151 1.273884 -0.000051
Cr -1.184649 -0.126513 0.000000
Cr 1.289974 0.098556 0.000001

$Ti_2H_6.H_2$, -1703.089299, *-83.7*, **-34.6**

H 0.043905 -0.961207 -0.883112
H 0.005932 0.067718 1.358135
H 2.752919 0.094895 0.834755
H -1.940589 -1.589391 -0.402140
H -0.212903 1.123894 -0.864606
H -2.252940 1.385886 -0.197054
Ti 1.201465 0.178840 -0.070652
Ti -1.309127 -0.045279 0.073563
H 2.289872 -1.358253 0.261892
H 1.682372 -1.701876 -0.171926

$V_2H_6.H_2$, -1892.152551, *-71.0*, **-21.7**

H -0.025086 0.000004 -1.282907
H -0.225267 -1.100506 0.763196
H 1.799323 -1.528986 0.018070
H -3.058090 -0.000003 -0.042698
H 1.799323 1.528986 0.018075
H -0.225266 1.100500 0.763204
V 1.114530 -0.000001 0.124450
V -1.331231 0.000000 -0.052173
H 2.459593 0.436199 -0.949658
H 2.459594 -0.436191 -0.949661

$Cr_2H_6.H_2$, -2093.110573, *-97.9*, **-50.2**

H -0.126408 0.547266 1.062817
H -0.126408 0.547271 -1.062815
H 2.722322 -0.658492 0.000001
H -2.550495 1.114376 0.000000
H 2.159093 -1.363938 0.000001
H 0.041270 -1.345599 -0.000002
Cr 1.125517 -0.000743 0.000000
Cr -1.383075 -0.068082 0.000000
H 2.403459 1.170194 0.000001
H 1.658558 1.640724 0.000001

$Ti_2H_6.6H_2$, -1709.004766, *-51.7*, **-7.1**

H 0.035535 -1.188005 0.606477
H -0.013978 0.330542 -1.289482
H -2.415175 0.078681 -1.543525
H 2.460596 0.227550 -1.372481
H -2.145705 0.922407 1.257937
H 0.089743 0.934488 0.973989
Ti -1.263365 0.006334 0.021750
Ti 1.324260 -0.007056 -0.011401
H -2.215339 -0.739308 -1.416114
H -1.531134 -1.619323 -0.626101
H 2.131366 -1.399773 -1.079274
H 1.767615 -1.858630 -0.515729
H -1.541502 1.785239 -0.683394
H -1.892816 1.784665 0.071695
H 1.843375 1.869220 0.153378
H 2.207743 1.611254 -0.533203
H 2.265828 -0.725879 1.643959
H 2.297190 0.055922 1.772267
H -2.428486 -0.688916 1.395439
H -2.254559 -1.364258 0.956477

$VH_6.5H_2$, -1896.898388, *-57.5*, **-13.0**

H	0.073638	0.995260	0.793805
H	0.073640	-0.995265	0.793800
H	-1.946877	-1.546533	-0.017275
H	2.752533	0.000004	-0.892004
H	-1.946869	1.546535	-0.017292
H	0.019481	-0.000001	-1.298669
V	-1.296130	-0.000001	-0.016982
V	1.275277	-0.000000	-0.027779
H	1.434484	-1.829158	-0.249040
H	2.078149	-1.516169	-0.661533
H	-2.720599	0.415919	-1.082445
H	-2.720602	-0.415919	-1.082442
H	1.434476	1.829159	-0.249038
H	2.078141	1.516173	-0.661531
H	-2.512918	0.405023	1.361359
H	-2.512921	-0.405006	1.361361
H	2.133075	0.000000	1.707294
H	2.762774	0.000002	1.223162

$Cr_2H_6.4H_2$, -2096.647881, *-50.6*, **-9.4**

H	-0.066179	-1.175385	-0.493269
H	-0.083427	0.959033	-0.768456
H	-2.489142	-1.057389	0.686390
H	2.498375	0.177846	-1.199867
H	-1.746567	-1.299895	1.080970
H	-0.024356	0.076584	1.234068
Cr	-1.246971	-0.043649	0.010903
Cr	1.287827	-0.034984	-0.068483
H	2.876327	-0.973723	0.106709
H	2.522844	-1.238730	0.782029
H	-2.655248	-0.140317	-1.036347
H	-2.080992	0.333486	-1.477459
H	-1.827737	1.744158	0.315057
H	-2.395016	1.333102	0.700093
H	2.471425	1.554807	0.409171
H	2.019160	1.593608	1.042830

Table S5. Cartesian Coordinates of $MH_3.nH_2$ (M = Ti and V) Pentamers, M_5H_{15}, and Cr_5H_{11} Optimized Geometry: SCF Energy, *Hydrogen Binding Energy (kJ mol^{-1}),* **Hydrogen Binding Gibbs Free Energy (kJ mol^{-1})**

Ti_5H_{15}, -4255.009824

H	0.616925	-2.106026	-0.451864
H	3.570351	-2.076910	0.228870
H	2.765892	0.455755	-1.104815
H	-1.866154	-1.708257	0.734078
H	0.690009	2.433852	-0.702304
H	0.116293	1.030246	1.131197
H	2.569181	2.120298	1.640230
H	-1.248076	-0.444307	-0.894337
H	-1.688759	0.431201	0.950595
H	-3.313508	-0.931714	-1.737272
Ti	-2.974940	-0.500579	-0.099914
Ti	-0.160912	-0.843116	0.723735
Ti	2.271349	-1.260464	-0.585325
Ti	1.817486	1.292726	0.299148
Ti	-0.844983	1.331841	-0.449158
H	-4.048741	0.494380	0.815311
H	0.619714	0.136411	-0.785995
H	1.761878	-0.519593	1.041614
H	-0.247866	-0.875880	2.447569
H	-2.673141	1.111572	-0.859559

V_5H_{15}, -4727.642867 **

H	-0.789724	-1.829317	1.214160
H	-2.625922	-1.926411	-1.423450
H	-2.605892	0.024332	1.092012
H	2.314935	-1.759280	0.160128
H	-0.673880	1.870882	1.064100
H	-0.741853	2.074867	-1.092571
H	-2.486594	1.833680	1.483694
H	1.276085	0.085868	1.122405
H	1.315747	-0.098927	-1.094586
H	3.265058	0.311909	1.551309
V	2.834692	-0.014512	-0.014967
V	0.568989	-1.316119	0.124261
V	-2.006525	-1.275821	-0.036896
V	-1.991974	1.292926	0.015584

V 0.585908 1.315159 -0.100045
H 3.842516 -0.192617 -1.342242
H -0.718232 -0.016156 -0.351286
H -2.807329 0.000490 -0.996050
H 2.335137 1.728678 -0.212254
H -0.695133 -2.145555 -0.897908

Cr_5H_{11}, -5227.651516 **

H 1.190866 -2.101911 -0.217435
H 3.266624 -1.759718 1.231991
H 2.915649 0.846116 0.235615
H -1.070627 -2.196935 -0.057827
H -0.087912 2.182657 -0.965643
H 1.002127 -0.285967 0.978757
H -0.099398 2.094536 1.079667
H -1.271891 -0.098574 -1.191653
H -0.978215 -0.267128 0.978590
Cr -2.484318 -1.066688 0.138934
Cr 0.005991 -0.834480 -0.271979
Cr 2.508511 -0.901806 0.060696
Cr 1.204213 1.453788 0.029155
Cr -1.363500 1.389177 -0.004241
H 1.269016 -0.024713 -1.205572
H -3.037777 0.651874 0.271950

$Ti_5H_{15}.5H_2$, -4260.921116, *-43.1*, **-1.9**

H 0.265086 -1.823614 -0.826038
H 3.189397 -2.451828 0.447047
H 2.931190 0.190065 -0.908735
H -1.886033 -1.668439 0.712908
H 0.843377 2.467745 -0.840455
H 0.203257 1.114373 1.077097
H 2.304237 1.951820 1.776534
H -1.193166 -0.347893 -0.940369
H -1.641116 0.524553 0.935567
H -3.153713 -1.486493 -1.508221
Ti -2.913930 -0.420908 -0.151305
Ti -0.233024 -0.806306 0.607005
Ti 2.043960 -1.438668 -0.409987
Ti 1.892311 1.266380 0.200559
Ti -0.747208 1.527685 -0.490333
H -3.789766 -0.216809 1.338151
H 0.659098 0.203966 -0.812231
H 1.699046 -0.393548 1.094930

H -0.446897 -0.809703 2.684782
H -2.603440 1.313569 -0.851273
H 2.965544 -3.011620 -1.136995
H 2.535069 -2.871619 -1.805006
H -1.165613 3.135992 0.668645
H -1.747705 3.211601 0.147440
H 3.328036 2.468286 0.651310
H 3.504911 2.382310 -0.143090
H -4.256373 -1.711299 -0.319242
H -4.411026 -1.356656 0.446263
H 0.886313 -2.241899 0.917232
H 0.053897 -1.392871 2.563088

$V_5H_{15}.5H_2$, -4733.574254, *-53.6*, **-11.1**

H 0.708371 1.780629 1.207542
H 2.782661 2.200349 -1.186757
H 2.605657 0.010622 1.042647
H -2.375318 1.592888 -0.397768
H 0.872408 -1.657646 1.192607
H 0.759553 -2.158064 -0.992648
H 2.998544 -1.997388 1.069610
H -1.407464 -0.103084 1.112363
H -1.240378 -0.078423 -1.027004
H -3.572441 0.450864 1.333476
V -2.864462 -0.072550 -0.084154
V -0.622496 1.332068 0.051995
V 1.970308 1.336053 -0.010208
V 2.061036 -1.251906 -0.092755
V -0.543253 -1.453021 0.084827
H -3.499339 -0.180276 -1.636167
H 0.654279 -0.015590 -0.247969
H 2.658756 0.097324 -1.121583
H -1.399269 3.151576 0.228038
H -2.230770 -1.779081 -0.409830
H -0.702855 -2.919520 1.298964
H -1.401419 -2.958200 0.914612
H 3.082870 2.751175 0.167500
H 2.886327 2.608356 0.976595
H 3.483290 -2.330766 -0.291534
H 3.281400 -2.184637 -1.103001
H 0.650929 2.051268 -1.009826
H -0.791697 3.182834 0.727305
H -4.453503 0.609617 0.106836
H -4.376666 0.390373 -0.797225

$Cr_5H_{11}.5H_2$, -5233.562326, *-46.0*, -**2.8 ****

H	1.451771	-2.072772	-0.001060
H	4.369920	-0.543278	0.018670
H	2.985845	0.857431	-0.007174
H	-1.329557	-2.187673	-0.004887
H	-0.074971	1.881150	-1.038635
H	1.321925	-0.151504	1.019015
H	-0.069657	1.874689	1.038652
H	-1.396548	-0.219903	-1.099761
H	-1.393535	-0.226727	1.099202
Cr	-2.566746	-0.948782	-0.000271
Cr	0.025049	-0.950426	-0.002651
Cr	2.740992	-0.881733	0.000824
Cr	1.266199	1.367950	-0.003782
Cr	-1.356096	1.339072	0.002209
H	1.323412	-0.154492	-1.024122
H	-3.056948	0.756051	0.004049
H	-3.284455	-1.308733	1.512506
H	-3.881069	-1.582853	0.931243
H	-1.524845	3.154855	0.020399
H	-2.295875	2.897414	0.013894
H	4.121986	-1.930617	0.020891
H	3.460242	-2.506289	0.015427
H	2.288574	2.912961	-0.001572
H	1.541126	3.212247	0.004512
H	-3.295947	-1.305844	-1.509368
H	-3.886962	-1.582047	-0.923795

$Ti_5H_{15}.10H_2$, -4266.798275, *-34.1*, **6.1 ****

H	-0.495562	-2.170762	0.438092
H	-3.864976	-1.579629	0.304232
H	-2.942771	0.437574	0.623022
H	1.953901	-1.787433	-0.534501
H	-0.706988	2.429006	0.353844
H	-0.053142	0.856765	-1.269488
H	-1.840224	2.654538	-1.644925
H	1.212203	-0.428525	0.913068
H	1.688822	0.362860	-1.008559
H	3.045359	-1.421811	1.600977
Ti	2.966194	-0.406547	0.181799
Ti	0.276269	-0.975666	-0.748567
Ti	-2.139941	-1.259805	0.584558
Ti	-1.803398	1.229904	-0.586171
Ti	0.819729	1.339099	0.395417

H 4.093726 0.742712 -0.518953
H -0.706095 0.177324 0.708149
H -1.626001 -0.674759 -1.153933
H 0.468151 -0.934622 -2.494647
H 2.591115 1.219750 1.008083
H -3.111861 -2.782775 0.031298
H -2.344082 -3.120184 0.046398
H 1.342148 2.995818 -0.721950
H 2.028854 2.825995 -0.395307
H -3.020578 2.753881 -0.449685
H -3.300436 2.310922 0.163188
H 4.385902 -0.730123 1.375145
H 4.718457 -0.144533 0.862534
H -3.037928 0.645408 -2.078715
H -2.744801 1.349404 -2.317548
H 0.355989 2.223320 2.211680
H 0.888828 1.693527 2.424699
H -2.074955 1.242296 3.738371
H -2.135534 1.161666 2.990165
H -3.153772 -1.871763 2.230553
H -2.438098 -1.824817 2.556194
H -0.014406 -2.744589 -1.449612
H 0.167711 -2.257214 -2.116620
H 3.854586 -1.368349 -1.326458
H 4.201698 -0.634525 -1.293596

$V_5H_{15}.10H_2$ -4739.426703, *-32.9*, **4.7** **

H -0.479456 -1.603485 0.996012
H -3.554134 -2.154684 0.177457
H -3.109011 0.408245 0.638560
H 1.323110 -1.967747 -0.417911
H -0.414135 2.467533 0.209732
H -0.224694 0.859572 -1.217691
H -2.477807 2.815316 0.213421
H 1.069596 -0.197346 0.817776
H 1.469366 -0.066590 -1.224850
H 2.623495 -2.091888 1.127402
V 2.648351 -0.858100 0.004849
V -0.024771 -0.802175 -0.500625
V -2.224395 -1.179453 0.590863
V -1.786266 1.331609 -0.252660
V 1.149830 1.538650 -0.069278
H 3.793371 -0.377134 -1.118240
H -0.823992 0.198329 0.816379
H -1.785580 -0.396797 -1.044617

H -0.058100 -1.084295 -2.331891
H 2.863350 0.924058 0.086176
H -1.176420 2.002810 2.711518
H -0.920809 1.902480 3.415342
H -3.143352 -2.327351 1.683439
H -2.599897 -2.030114 2.240820
H -2.510217 2.636013 -1.248582
H -2.236781 2.112750 -1.863843
H -1.021379 -2.234954 -0.506792
H -0.170385 -1.829356 -2.020011
H 3.488999 -2.387598 -0.388955
H 3.845022 -1.794603 -0.912779
H 1.293451 2.733568 1.412858
H 2.035193 2.436250 1.374751
H 3.751737 -0.977610 1.454834
H 4.038501 -0.288929 1.100087
H 1.304680 3.164967 -1.093357
H 2.025140 2.840744 -1.186024
H -3.059187 -2.419239 -3.183462
H -3.105290 -2.285694 -2.442324
H 1.769912 0.309429 3.808344
H 1.632493 0.001125 3.133973

$Cr_5H_{11}.10H_2$, -5239.407266, *-25.5*, **6.6 ****

H 1.376138 -2.191117 0.188549
H 4.329215 -0.730548 0.150968
H 2.980556 0.692665 -0.033160
H -1.406259 -2.244528 0.122099
H -0.028780 1.689085 -1.229634
H 1.268405 -0.185272 1.033334
H -0.073676 1.865015 0.839720
H -1.399088 -0.379549 -1.141688
H -1.449224 -0.193240 1.048807
Cr -2.612777 -0.983032 -0.013737
Cr -0.022480 -1.042052 0.051750
Cr 2.693457 -1.033247 0.120174
Cr 1.274221 1.239317 -0.119259
Cr -1.347386 1.268930 -0.179284
H 1.319046 -0.367762 -1.001009
H -3.061433 0.725986 -0.171012
H -3.375249 -1.192780 1.505410
H -3.964160 -1.503674 0.934897
H -1.472419 3.082570 -0.324030
H -2.249087 2.842624 -0.328187
H 4.047712 -2.106521 0.267767

H 3.372519 -2.665709 0.295272
H -0.133205 -0.156680 -4.257494
H -0.273026 -0.126044 -3.517986
H 2.333431 2.755619 -0.225171
H 1.593535 3.070698 -0.264757
H 2.558081 1.942135 -3.262414
H 1.858353 1.733729 -3.073275
H 2.831193 1.808337 2.452275
H 2.579591 2.290550 2.975008
H -0.101275 0.793815 3.344112
H -0.089507 0.795092 4.097210
H -3.313855 -1.455110 -1.504453
H -3.925335 -1.665700 -0.912653
H -2.889059 1.853109 2.434338
H -2.883966 2.425217 2.925685

$Ti_5H_{15}.9H_2$, -4265.629581, *-37.1*, **4.7 ****

H -0.540329 -2.171801 0.376599
H -3.903855 -1.533843 0.373564
H -2.945839 0.450639 0.780054
H 1.885879 -1.762595 -0.642622
H -0.691710 2.427429 0.560532
H -0.104976 0.943116 -1.167825
H -1.877364 2.780625 -1.388735
H 1.203519 -0.480129 0.900709
H 1.636767 0.414338 -0.985645
H 3.041614 -1.532987 1.477940
Ti 2.936462 -0.437193 0.121743
Ti 0.214056 -0.919953 -0.761784
Ti -2.167467 -1.251196 0.621926
Ti -1.830177 1.297322 -0.414322
Ti 0.820669 1.318808 0.496054
H 4.059374 0.736812 -0.544562
H -0.711386 0.159293 0.785870
H -1.694578 -0.573654 -1.094488
H 0.357462 -0.781205 -2.507488
H 2.606752 1.143436 1.049738
H -3.175051 -2.728263 0.011017
H -2.411792 -3.075112 -0.015205
H 1.333958 3.030490 -0.539719
H 2.027186 2.834053 -0.243159
H -3.022300 2.825375 -0.156330
H -3.290845 2.351390 0.438118
H 4.384546 -0.845525 1.253407
H 4.710504 -0.235527 0.765623

H -3.113859 0.814077 -1.901609
H -2.818033 1.527058 -2.108296
H 0.420037 2.102958 2.372304
H 0.951412 1.555514 2.539398
H -3.142962 -1.944344 2.258875
H -2.417872 -1.924672 2.565946
H -0.120087 -2.642203 -1.553773
H 0.049848 -2.119611 -2.196906
H 3.769123 -1.321504 -1.463758
H 4.126927 -0.594959 -1.399157

$V_5H_{15}.7H_2$, -4735.922841, *-44.6*, **-1.3 ****

H 0.498841 -1.748131 -0.803566
H 3.415541 -2.434767 0.097389
H 3.099682 0.276667 -0.658880
H -1.402652 -1.870737 0.532553
H 0.616671 2.323619 -0.685953
H 0.198970 1.014706 1.080092
H 2.113275 2.982213 0.376017
H -1.037578 -0.282258 -0.893905
H -1.497952 0.113746 1.125097
H -2.693830 -2.129407 -0.989961
V -2.663865 -0.756690 -0.039628
V -0.004700 -0.748975 0.556226
V 2.243986 -1.318197 -0.423065
V 1.823477 1.299035 0.175783
V -1.013459 1.535643 -0.293067
H -3.814903 -0.040578 0.944533
H 0.870483 0.097653 -0.822488
H 1.759348 -0.294853 1.092220
H -0.120795 -0.852011 2.396307
H -2.768745 1.000860 -0.386499
H 3.238463 -2.405776 -1.522992
H 2.809303 -2.001728 -2.102161
H 2.799444 2.280164 1.268998
H 2.964616 1.451703 1.550530
H 0.989048 -2.156683 0.812255
H 0.176831 -1.584299 2.179571
H -3.564056 -2.166290 0.619367
H -3.906210 -1.480367 1.010898
H -1.134790 2.391259 -1.997136
H -1.888115 2.143528 -1.887057
H -3.751640 -1.050884 -1.465723
H -4.023727 -0.307538 -1.214187
H -1.037692 3.363014 0.359925

H -1.772898 3.118413 0.531048

$Ti_5H_{15}.15H_2$, -4272.6407121, *-25.0*, **9.5 ****

H 0.555077 -2.148837 0.258271
H 3.906705 -1.503196 0.144109
H 2.953363 0.275680 -0.834401
H -1.882103 -1.502307 1.076290
H 0.680900 2.206198 -1.229089
H 0.067949 1.268086 0.832941
H 1.818756 3.114197 0.565050
H -1.172247 -0.704101 -0.756143
H -1.668974 0.684963 0.773075
H -2.949102 -1.915722 -1.066172
Ti -2.924093 -0.481189 -0.070257
Ti -0.222598 -0.633784 0.979060
Ti 2.177019 -1.319538 -0.215549
Ti 1.806462 1.416694 0.044600
Ti -0.827694 1.142428 -0.882891
H -4.089111 0.807151 0.183850
H 0.720626 -0.029117 -0.801606
H 1.671651 -0.181460 1.223188
H -0.393692 0.000080 2.608813
H -2.592662 0.772776 -1.405308
H 3.182165 -2.560606 0.789059
H 2.419142 -2.898290 0.893325
H -1.403283 3.050748 -0.355407
H -2.043768 2.812694 -0.729681
H 2.996906 2.825098 -0.612134
H 3.280203 2.206447 -1.043087
H -4.332777 -1.231856 -1.078867
H -4.682143 -0.519956 -0.792538
H 3.066476 1.387135 1.630091
H 2.757999 2.123771 1.626006
H -0.377123 1.348958 -2.897961
H -0.917117 0.785628 -2.913286
H 2.098711 0.011605 -4.032390
H 2.152947 0.174307 -3.297154
H 3.161767 -2.446738 -1.597773
H 2.436333 -2.521038 -1.890035
H 0.114743 -2.055315 2.233873
H -0.071050 -1.376186 2.699361
H -3.785049 -0.864349 1.686389
H -4.155164 -0.200936 1.395842
H -0.457257 -2.062269 -2.766189
H -0.097183 -2.123362 -3.425701

H -2.397762 1.427496 3.188548
H -2.975670 1.791540 3.506588
H -1.445601 -3.900854 -0.867078
H -1.164677 -4.586960 -1.002145
H -0.906283 3.919673 2.298279
H -0.280817 3.703434 1.935048
H 2.861820 -0.979063 3.175139
H 3.136266 -1.126579 3.861823

$V_5H_{15}.13H_2$, -4742.9317271, *-26.8*, **7.8 ****

H -0.450224 -1.778194 0.606475
H -3.488379 -2.217184 -0.367565
H -3.125463 0.201408 0.647501
H 1.371187 -1.799676 -0.830911
H -0.487199 2.375080 0.660324
H -0.246620 1.088056 -1.042139
H -2.545032 2.708110 0.649207
H 1.070204 -0.336865 0.742062
H 1.467330 0.233223 -1.228996
H 2.695015 -2.210895 0.644072
V 2.669012 -0.765847 -0.189346
V -0.006276 -0.675976 -0.683078
V -2.201745 -1.320818 0.282630
V -1.826161 1.322441 -0.032236
V 1.102213 1.550160 0.236275
H 3.785767 -0.019422 -1.188140
H -0.834024 0.024373 0.800291
H -1.774871 -0.206980 -1.150004
H -0.020375 -0.572698 -2.534388
H 2.829937 0.962057 0.281863
H -1.640322 2.179142 2.946352
H -1.470744 2.046707 3.671147
H -3.085150 -2.714694 1.094026
H -2.557706 -2.529134 1.705385
H -2.584371 2.744614 -0.815371
H -2.311861 2.319134 -1.503917
H -0.968364 -2.097616 -0.996832
H -0.126024 -1.367044 -2.385151
H 3.544737 -2.150567 -0.912288
H 3.876288 -1.449943 -1.298551
H 1.185079 2.419365 1.934070
H 1.936012 2.155587 1.853182
H 3.812676 -1.158325 1.181190
H 4.075016 -0.404555 0.973025
H 1.234585 3.356040 -0.426382

H 1.962805 3.071596 -0.571613
H -2.962361 -1.731706 -3.695451
H -3.021838 -1.767985 -2.944197
H 2.297130 -0.224186 3.762798
H 2.006756 -0.457648 3.107521
H -1.085483 -0.668671 3.230279
H -0.792389 -1.018275 3.830555
H 0.447100 2.674715 -3.633709
H 0.185917 2.346028 -3.007620
H 1.059717 -3.104800 2.235956
H 0.783559 -3.447230 2.848326

$Cr_5H_{11}.12H_2$, -5241.7452274, *-22.6*, **9.1** **

H 1.422066 -2.045276 0.271732
H 4.217957 -0.291517 0.413121
H 2.855373 0.881095 -0.256535
H -1.392023 -2.239559 0.329459
H -0.208582 1.579752 -1.418596
H 1.272127 0.004995 1.005949
H -0.269676 1.960568 0.630687
H -1.489166 -0.514665 -1.130887
H -1.544331 -0.106282 1.039970
Cr -2.655129 -1.055173 0.059688
Cr -0.051782 -0.994036 0.131388
Cr 2.675999 -0.815560 0.129390
Cr 1.117170 1.341109 -0.279319
Cr -1.512186 1.221030 -0.326559
H 1.265088 -0.337547 -0.991228
H -3.197759 0.604982 -0.267099
H -3.400452 -1.158761 1.601020
H -3.957392 -1.584134 1.073474
H -1.696309 3.002190 -0.638502
H -2.465988 2.734265 -0.626695
H 3.934297 -1.692205 1.026832
H 3.303091 -2.251338 1.050066
H 0.720527 -2.079637 -3.676960
H 0.506915 -1.722359 -3.048696
H 2.066247 2.898225 -0.587638
H 1.302982 3.159006 -0.618046
H 2.248043 1.229724 -3.817101
H 1.849400 1.011842 -3.214176
H 2.661515 2.297104 2.169312
H 2.208440 2.772977 2.540197
H -0.308865 1.221238 3.183597
H -0.193818 1.260885 3.927152

H -3.299824 -1.730841 -1.374391
H -3.895744 -1.938273 -0.762473
H -3.133153 2.006040 2.193244
H -3.180299 2.608420 2.644446
H 3.799761 -1.446379 -1.498587
H 3.171800 -1.881987 -1.628531
H 2.713503 -0.569987 3.964926
H 2.336519 -0.379458 3.340841